



Figure S1. Predictive performance assessment of PBPK models that have prospective predictions (including Shuno et al. 2009¹ and Shuno et al. 2010²). a) Predicted AUCR vs. Observed AUCR. b) Predicted C_{max}R vs. Observed C_{max}R. c) Predicted t_{max}R vs. Observed t_{max}R. Red solid lines in all plots are lines of identity ($y = x$). Red dashed lines in all plots represent $y = 0.8x$ and $y = 1.25x$. Pink dotted lines in all plots represent $y = 0.5x$ and $y = 2x$. Blue dashed lines in all plots represents $y = 1.25$ and $x = 1.25$.

Reference

1. Shono Y. et al. Prediction of food effects on the absorption of celecoxib based on biorelevant dissolution testing coupled with physiologically based pharmacokinetic

- modeling. *Eur J Pharm Biopharm.* **73**, 107-114 (2009).
2. Shono Y., Jantratid E., Kesisoglou F., Reppas C., Dressman J.B.. Forecasting in vivo oral absorption and food effect of micronized and nanosized aprepitant formulations in humans. *Eur J Pharm Biopharm.* **76**, 95-104 (2010).